METHOD, SYSTEM, AND COMPUTER PROGRAM PRODUCT FOR DETERMINING PROPERTIES OF COMBINATORIAL LIBRARY PRODUCTS FROM FEATURES OF LIBRARY BUILDING BLOCKS

ABSTRACT

The present invention determines properties of combinatorial library products from features of library building blocks. At least one feature is determined for each building block of a combinatorial library having a plurality of products. A training subset of products is selected from the products, and at least one property is determined for each product of the training subset. A building block set is identified for each product of the training subset, and an input features vector is formed from the features of the identified building blocks for each product of the training subset. A supervised machine learning approach is used to infer a mapping function that transforms the input features vector for each product of the training subset to the corresponding at least one property for each product of the training subset. After the mapping function is inferred, it is used for determining properties of other products of the library from their corresponding input features vectors.